

As a general comment on my assessment of the fibre diffraction part of the meeting, it was very clear that even on an international scale the fibre diffraction community is relatively small compared with, say, our macromolecular crystallography colleagues. On the other hand, we still have a great deal to learn about getting our act together, about cooperating and informing each other of what is going on and in making sure that internationally we really are a community. Of key importance for the good of our subject is

therefore the need not only to advertise organisations such as CCP13 as widely as possible, something that I tried to do, of course, in Montreal, but also for CCP13, the ACA SIG and other groups in other countries to coordinate their efforts in some way in order to promote as fully as possible what is a very important area of study.

John Squire

4th Annual CCP13/NCD Workshop

The fourth annual workshop for the collaborative computational project for fibre diffraction (CCP13) and non-crystalline diffraction (NCD) was held at Daresbury on the 9th-11th of May attracted 75 participants. The meeting was partially sponsored by Q-Associates, Siemens and Organised Computer Systems.

To reflect the joint nature of the workshop a diversity of topics, including synthetic polymers, hardware sources and detectors, software developments and biological systems, were covered. Each session began with an eminent keynote speaker, followed by presentations from specialists in the field, which included participants from not only the UK but also Belgium, France, Germany, Holland and the USA. A new feature this year was a series of short presentations (no more than 3 minutes), by students, on the content of their posters. The talks were complemented by a poster session and a commercial exhibition by the sponsors Q-Associates, Siemens and Organised Computer Systems.

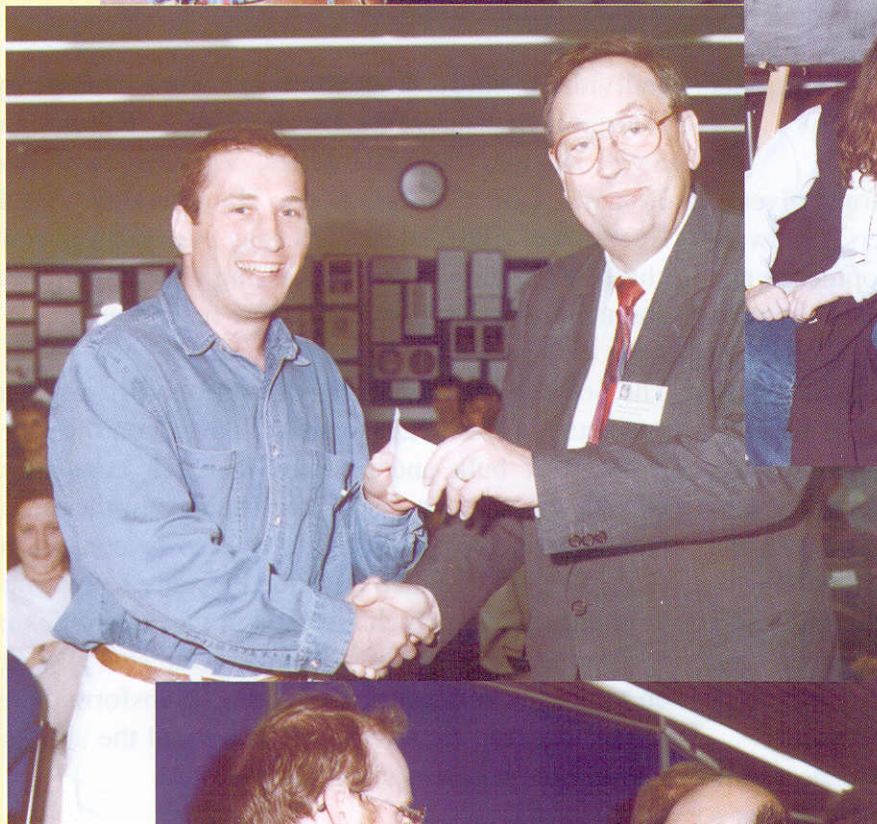
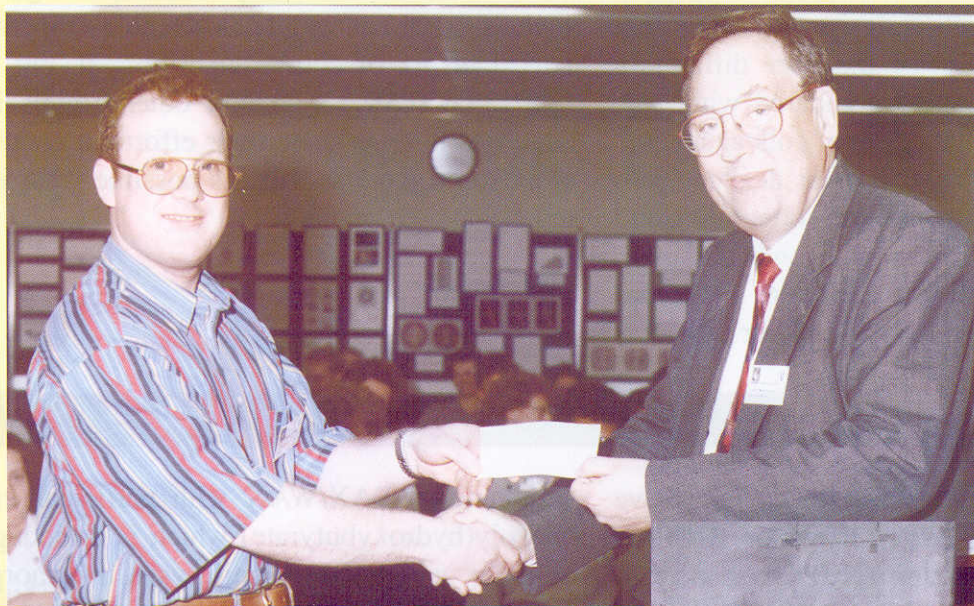
After the Chairman's introduction G.Zachmann (Hamburg) opened the polymer session by giving a general introduction to polymers, before going on to describe work on spinning/extrusion of polypropylene, SAX/WAX studies of polyvinylidene fluoride, liquid crystalline polymer dislocations studied on the micro-focus beamline at the ESRF and grazing incidence (30Å depth into layer) studies of PET films. B.Komanschek (Daresbury) then described the current facilities, for polymer studies, available at the SRS, primarily on stations 8.2 and 16.1. A.Ryan (UMIST) described his latest work on the time resolved SAX/DSC crystallisation block copolymers, in particular PBO-PEO and PEE-PE head to tail polymers where only half crystallises. R.Cameron concluded the session with a talk on the phase transitions of natural polymers studied by

simultaneous SAX/WAX with particular emphasis on Poly(hydroxybutyrate) which is a biodegradable polymer which has semi-crystalline morphology (spherulite).

Individual short presentations were made by Georgina Bryant, Mike Ewell, Patrick Fairclough, Steve Naylor, Catherine Miles, V. Balaguraswamy, Richard van Gelder, Andy Hammersley, Mark Boehm and Alun Ashton. Tuesday evening was concluded with dinner, poster viewing and judging, the commercial exhibition and a wine reception.

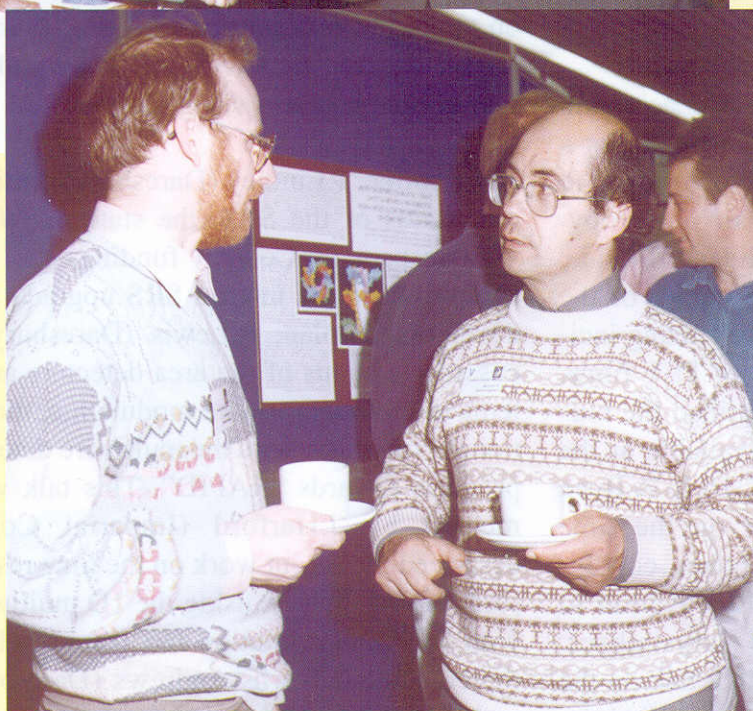
The second day commenced with another keynote presentation from H.Reynaers (Leuven) on the morphology of bulk and oriented tri-block copolymer gels in which he described the changes in the structure on stretching from a spherical to layered form. G.Tiddy (Salford) then described a study of lyotropic liquid crystals which are used in vast quantities in the surfactant industry. E.Pantos (Daresbury) went on to discuss his recent work on gel transformations studied by SAXS, SANS and NMR and the simulation of the processes using fractals.

After coffee, P.Lindley (Daresbury) outlined the current status of the SRS, the state of NCD research with respect to Council funding, the strategy for Diamond and the interim SRS upgrade and detector development plan. R.Lewis (Daresbury) then discussed the status of the area detectors and the problems of the detector wire modulation, the first operational experience with the multiwire detector, and the progress towards "RAPID". This talk was complemented by J.Harford (Imperial College) who described the recent work on the time resolved X-ray study of fish muscle using the 1D multiwire detector with 1ms time resolution and 1mm resolution across the equator. E.Towns-Andrews (Daresbury) continued the hardware theme with a talk on recent results



Top and Centre Left: Mike Elwell and Richard Denny (on behalf of Jeff Harford) receive cheques as joint winners of the prize for best poster from Gerhard Zachmann

Centre Right: Anthony Gleeson points out his favourite dish on the evening menu to Catherine Miles.



Bottom: Goran Ungar and Rob

and developments on SRS station 16.1, highlighting in particular three experiments: firstly, the 20mS time resolved studies of muscle by M.Ferenczi, secondly, the slitted beam work of J.Squire utilising an A3 image plate to record the 59Å reflection of fish muscle and lastly the insect flight muscle work of M.Reedy. M.Lorenzen (ESRF) then described the development of a high pressure cell for use on the micro-focus and high brilliance beamlines at the ESRF, highlighting its use with recent results on tri-block gels. T.Irving (Chicago) rounded up the session by outlining the plans for the BioCAT (Collaborative Access Team) beamline at the Advance Photon Source.

After coffee the poster prizes were awarded. The judges (P.Lindley and G.Zachmann) deliberation was to award a joint first place prize to J.Harford *et al* (Imperial College, London), a cheque for £75, for their poster "Muscle the Movie", and for the second year in succession to M.Elwell (UMIST) for his poster "Simultaneous SAXS/FTIR".

R.Rule (ICI) opened a short session on software by describing the modelling of SAXS patterns of polyurethane utilising correlation functions. He also stressed the importance of error correction, with particular reference to beam intensity measurements and scaler overflow. R.Denny (Daresbury/Imperial College) then described the progress on the CCP13 program suite, outlining the developments in the programs FIX, TBACK, LSQINT, SAMPLE and DECONV.

J.Bordas (Liverpool) discussed the effect of the anti-tumor drug, taxol, on the assembly of tubulin as studied by turbidity and SAXS and also the effect of vinblastin as observed by cryoelectron microscopy (EM), highlighting the relationship between EM and

SAXS. C.Blake (Oxford) finished the afternoon with a talk on amyloidosis caused by an aggregation of proteins to form fibrils, as studied by X-ray diffraction, which have been implicated in diseases such as Alzheimers, type II diabetes and BSE. The second day concluded with a sherry reception and conference dinner at Daresbury.

The final day started with M.Reedy discussing his latest work, hot from the beamline, on the time resolved structure of insect flight muscle contraction, complementing this with electron microscopy studies. M.Ferenczi (NIMR) described some recent developments in the time resolved x-ray diffraction of single muscle fibres, using stepped length changes with stretch and release and also permeabilised fibres using alpha-toxin. D.Marvin (Cambridge) then outlined the maximum entropy method in the study of Filamentous Bacteriophage. The structure is rod like alpha-helix when magnetically aligned, multiple calculations were then performed selecting the best fits. W.Fuller (Keele) showed a video of the instrumentation and results of the development of crystallinity recorded on the micro-focus beamline at the ESRF. The meeting was rounded off with presentations from P.Langan on neutron studies on the D19 beamline at the ILL, S.Perkins (Royal Free Hospital) on the automated curve fitting of SAXS data of multidomain proteins and lastly W.Bras (AMOLF) on the magnetic alignment of microtubules.

The workshop concluded with a special vote of thanks to Val Matthews and Vanessa Porter for all the hard work and organisation that went into making the whole meeting run smoothly.

Geoff Mant

CCP13 and the World Wide Web

The huge growth of the Internet as a mechanism for the rapid dissemination of information has led to the creation of the CCP13 website. The CCP13 home page (Figure 1) is available from the URL:

<http://www.dl.ac.uk/CCP/CCP13>

The home page currently points to six areas of information, a general introduction, the committee, workshops, newsletters, software and publications. To date, all of the previous workshop abstracts and newsletters have been digitised and converted to WWW viewable documents. We hope that, from this

year on, submissions to the CCP13 workshop and contributions to the newsletters will be submitted electronically.

The latest addition to our pages is the CCP13 license form and program retrieval mechanism (see Figure 2). Basically, all subscribers are requested to enter their name and E-mail address and select the desired program and operating system on which it will run. Selection of the retrieve link on the subsequently displayed page will transfer a compressed executable version of the program to a directory you specify.